Jacob O. Spiegel, Ph.D.

Pittsburgh, PA jspiegel@pitt.edu (516) 984-7751 linkedin.com/in/jacob-spiegel-phd/

I am seeking to transition from academia to industry. I am self-motivated and a fast learner, and I love working on team-based collaborations.

With a Ph.D. in molecular biophysics, a Ph.D. minor in teaching, and a Bachelor of Engineering, I have a multi-disciplinary background. I have three years of computational biology, Python programming, and open-source tool-development experience, as well as ten years of wet lab experience. I hope to bring my diverse background in science, engineering, and communications to tackle interdisciplinary challenges.

Education

University of Pittsburgh 2014 – 2020
Ph.D in Molecular Biophysics and Structural Biology Pittsburgh, PA
- Thesis title: "Targeting the Poly (ADP-Ribose) Polymerase-1 Catalytic Pocket Using AutoGrow4, a Genetic Algorithm for *De Novo* Design"

Ph.D Minor in Teaching

Carnegie Mellon University 2013 – 2014
Ph.D. Student in Molecular Biophysics and Structural Biology Pittsburgh, PA

Stony Brook University 2009 – 2013
B.Eng. in Biomedical Engineering - Cellular and Molecular Biology Track Stony Brook, NY

Professional Experience

University of Pittsburgh 2013 – 2020
Ph.D. Candidate/Researcher in Dr. Jacob Durrant's laboratory Pittsburgh, PA
- Designed, developed, documented, and maintained multiple Python open-source programs for computer-aided drug designed (CADD) and cheminformatics; parallelized code for multiprocessing
- Applied CADD techniques to biological targets; performed molecular dynamic (MD) and weighted ensemble MD simulations on multiple proteins; performed protein homology modeling
- Completed independent and collaborative projects
- Authored scientific articles for publication
- Mentored, managed, and designed projects for/with undergraduate and graduate students

Ph.D. Candidate in Dr. Roger Hendrix's laboratory
- Studied bacteriophages using biochemical, molecular genetic, and X-ray crystallography techniques
- Engineered plasmids; designed protein purification protocols; purified proteins for X-ray crystallography

Stony Brook University 2011 – 2013
Undergraduate Researcher in Dr. Balaji Sitharaman's laboratory Stony Brook, NY
- Studied nanoparticle drug delivery system targeting cancer cells
- Designed alternative exfoliation protocol to produced graphene sheets from graphite

Publications

Peer-Reviewed Articles
- **Spiegel, J.O.**, Durrant, J.D. AutoGrow4: an open-source genetic algorithm for *de novo* drug design and lead optimization. J Cheminform 12, 25 (2020). http://doi.org/ggwwcp
- Ropp, P.J., **Spiegel, J.O.**, et al. Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. J Cheminform 11, 34 (2019). http://doi.org/gf48dh

Articles in Preparation
- **Spiegel, J.O.**, O'Donnell, A., Durrant, J.D., (2020). Molecular dynamics of α-arrestin TXNIP.
- **Spiegel, J.O.**, Durrant, J.D., (2020). Mechanism and Pharmaceutical Intervention of Poly (ADP-ribose) polymerase 1 (PARP-1).
- **Spiegel, J.O.**, Durrant, J.D., Bowman, R., O'Donnell, A. (2020). Putting the brakes on α-arrestin trafficking: α-arrestin regulation by phosphorylation and ubiquitination.